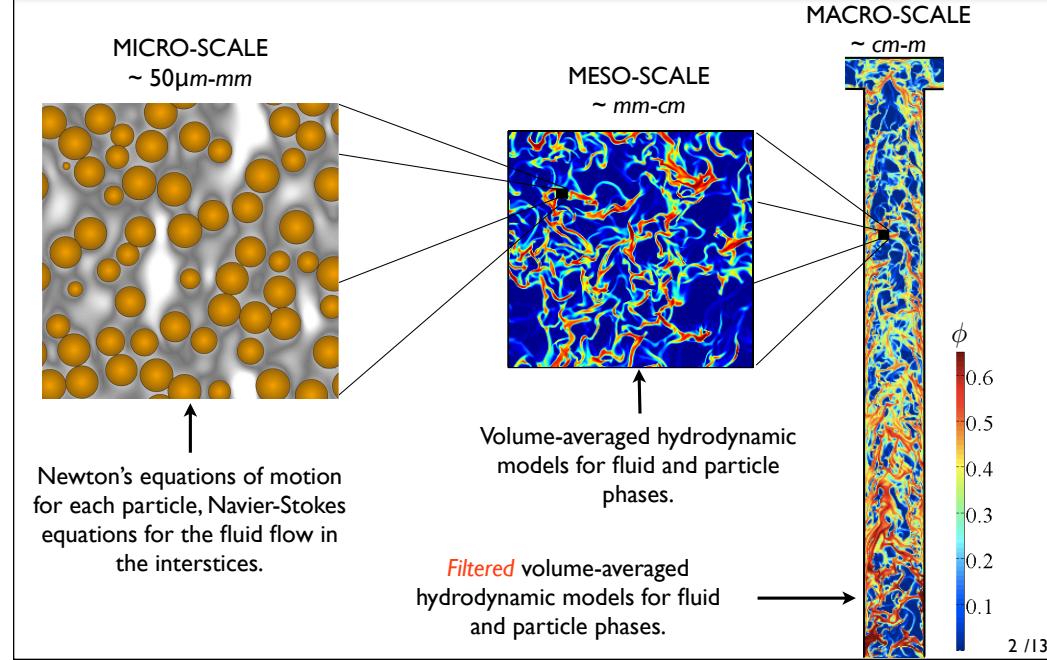




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Simulation of Gas-Particle Flows Across Length Scales



Development of Filtered Two-Fluid Models



- Hydrodynamics (*Igci et al, 2011*)
 - Filtered drag *
 - Filtered pressure
 - Filtered viscosity
- Reacting flows (*Holloway & Sundaresan, 2012*)
 - Filtered reaction rate
- Thermal energy & interphase transport (**present work**)
 - Filtered energy dispersion
 - Filtered interphase heat/mass transfer
 - Filtered scalar dispersion (**no interphase transport**)
 - Helium Tracer/Solid Particle Tracer

**Li & Kwauk, 1994; Parmentier et. al, 2011*

Two-Fluid Model Equations



Continuity

$$\frac{\partial(\rho_s \phi_s)}{\partial t} + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s) = 0$$

$$\frac{\partial(\rho_g \phi_g)}{\partial t} + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g) = 0$$

Momentum

$$\frac{\partial}{\partial t}(\rho_s \phi_s \mathbf{v}_s) + \nabla \cdot (\rho_s \phi_s \mathbf{v}_s \mathbf{v}_s) = -\nabla \cdot \boldsymbol{\sigma}_s - \phi_s \nabla \cdot \boldsymbol{\sigma}_g + \mathbf{f} + \rho_s \phi_s \mathbf{g}$$

$$\frac{\partial}{\partial t}(\rho_g \phi_g \mathbf{v}_g) + \nabla \cdot (\rho_g \phi_g \mathbf{v}_g \mathbf{v}_g) = -\phi_g \nabla \cdot \boldsymbol{\sigma}_g - \mathbf{f} + \rho_g \phi_g \mathbf{g}$$

Granular kinetic theory

Wen & Yu (1966)

Thermal Energy

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t}(\phi_s T_s) + \nabla \cdot (\phi_s \mathbf{v}_s T_s) \right] = \nabla \cdot (k_s \nabla T_s) + \gamma(T_s - T_g)$$

$$\rho_g C_{p_g} \left[\frac{\partial}{\partial t}(\phi_g T_g) + \nabla \cdot (\phi_g \mathbf{v}_g T_g) \right] = \nabla \cdot (k_g \nabla T_g) - \gamma(T_s - T_g)$$

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Gunn (1978)

Filtered Equations



Filter

$$\overline{\phi_s}(\mathbf{x}, t) = \int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \phi_s(\mathbf{x}, t) d\mathbf{y} \quad \int_{V_\infty} G(\mathbf{x}, \mathbf{y})(\mathbf{x}, t) d\mathbf{y} = 1$$

Favre Filter

$$\widetilde{\alpha_s}(\mathbf{x}, t) = \frac{\int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \alpha_s(\mathbf{x}, t) \phi_s(\mathbf{x}, t) d\mathbf{y}}{\int_{V_\infty} G(\mathbf{x}, \mathbf{y}) \phi_s(\mathbf{x}, t) d\mathbf{y}}$$

Filtered Solids Thermal Energy Equation

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t} (\widetilde{\phi_s T_s}) + \nabla \cdot (\widetilde{\phi_s v_s T_s}) \right] = \nabla \cdot (\overline{k_s \nabla T_s}) + \overline{\gamma(T_s - T_g)} + \rho_s C_{p_s} \nabla \cdot \left[\widetilde{\phi_s v_s T_s} - \overline{\phi_s} \widetilde{v_s T_s} \right]$$

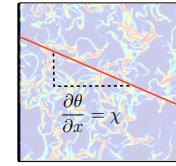
↑
'dispersive' flux

Applying Mean Temperature Gradient



Temperature Gradient

$$T_s = T'_s + \theta(x) \quad \frac{\partial \theta}{\partial x} = \chi = \text{constant}$$
$$T_g = T'_g + \theta(x)$$



Thermal Energy

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t} (\phi_s T'_s) + \nabla \cdot (\phi_s \mathbf{v}_s T'_s) \right] = \nabla \cdot (k_s \nabla T'_s) + \gamma(T'_s - T'_g) + \chi \frac{\partial k_s}{\partial x} - \rho_s C_{p_s} \phi_s v_{s_x} \chi$$

$$\rho_g C_{p_g} \left[\frac{\partial}{\partial t} (\phi_g T'_g) + \nabla \cdot (\phi_g \mathbf{v}_g T'_g) \right] = \nabla \cdot (k_g \nabla T'_g) - \gamma(T'_s - T'_g) + \chi \frac{\partial k_g}{\partial x} - \rho_g C_{p_g} \phi_g v_{g_x} \chi$$

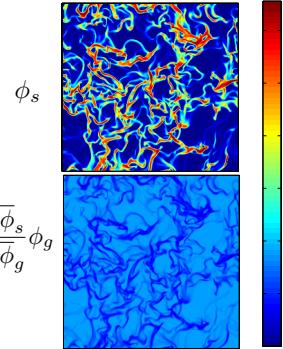
‘New’ source terms

Applying Heat Sources/Sinks



Solids Heat Source

$$\dot{Q}_s \phi_s \quad \int_D \dot{Q}_s \phi_s dV = \dot{Q}_s \bar{\phi}_s V$$



Gas Heat Sink

$$\dot{Q}_g \phi_g = \dot{Q}_s \frac{\bar{\phi}_s}{\phi_g} \phi_g \quad \int_D \dot{Q}_g \phi_g dV = \dot{Q}_s \bar{\phi}_s V$$

Thermal Energy

$$\rho_s C_{p_s} \left[\frac{\partial}{\partial t} (\phi_s T_s) + \nabla \cdot (\phi_s \mathbf{v}_s T_s) \right] = \nabla \cdot (k_s \nabla T_s) + \gamma(T_s - T_g) + \dot{Q}_s \phi_s$$

$$\rho_g C_{p_g} \left[\frac{\partial}{\partial t} (\phi_g T_g) + \nabla \cdot (\phi_g \mathbf{v}_g T_g) \right] = \nabla \cdot (k_g \nabla T_g) - \gamma(T_s - T_g) - \dot{Q}_g \phi_g$$

‘New’ source/sink terms

Simulations and Filtering Procedure



2-D periodic domain with mean vertical pressure drop in gas phase set to balance weight of mixture.

Computational Domain: 32cm x 32cm

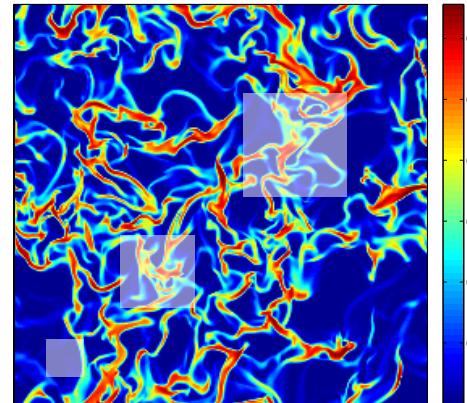
Discretization: 256 x 256 cells

Particle diameter: 75 μ m

Simulations are for FCC particles in air.
Results are suitably scaled so that they are
applicable to other systems.

Snapshot of solids volume fraction field
obtained from highly resolved simulations. →

Shaded squares illustrate regions over
which a filtering operation is performed.



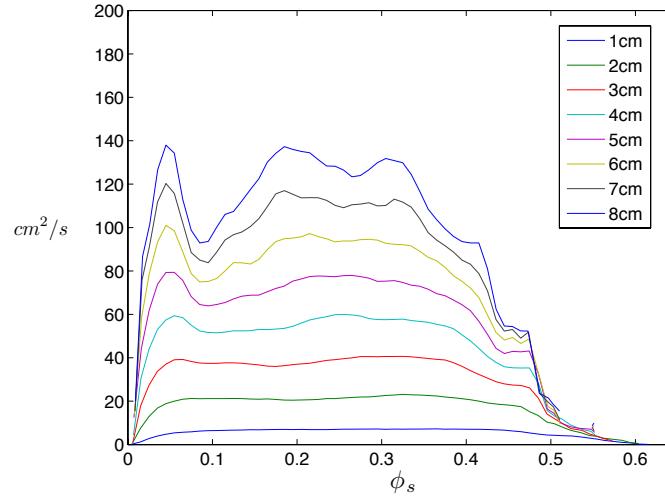
Filtered Solids Thermal Dispersion



$$\alpha_{filt} = \frac{k_{filt}}{\rho_s C_{p_s}} = \frac{\overline{\phi_s} \left(\widetilde{v_{sx} T_s} - \widetilde{v_{sx} T_s} \right)}{\frac{\partial \widetilde{T_s}}{\partial x}} = \frac{\left(\widetilde{v_{sx} T_s} - \widetilde{v_{sx} T_s} \right)}{\frac{\partial \widetilde{T_s}}{\partial x}}$$

Curves correspond to different filter sizes.

FCC particles in air.



Scaled Filtered Solids Thermal Dispersion



$$\frac{\alpha_{filt}}{(v_t^3/g)} = \overline{\phi_s} h(\overline{\phi_s}) (Fr_\Delta)^\delta$$

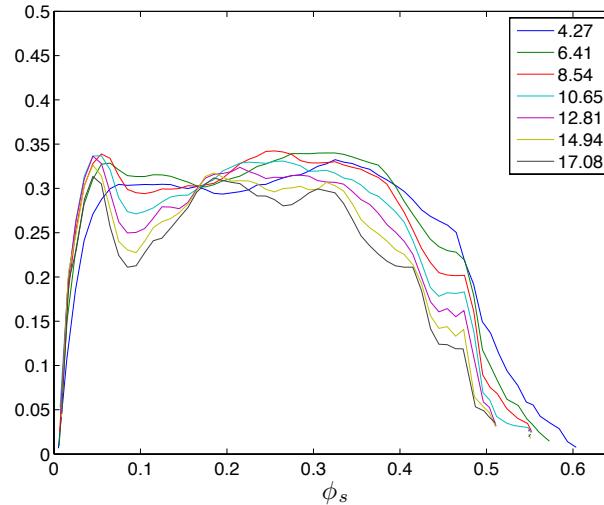
$$\delta = -4/3$$

Dimensionless filter size shown in legend $\frac{\Delta}{v_t^2/g}$

\uparrow

$(Fr_\Delta)^{-1}$

$$h(\overline{\phi_s})$$



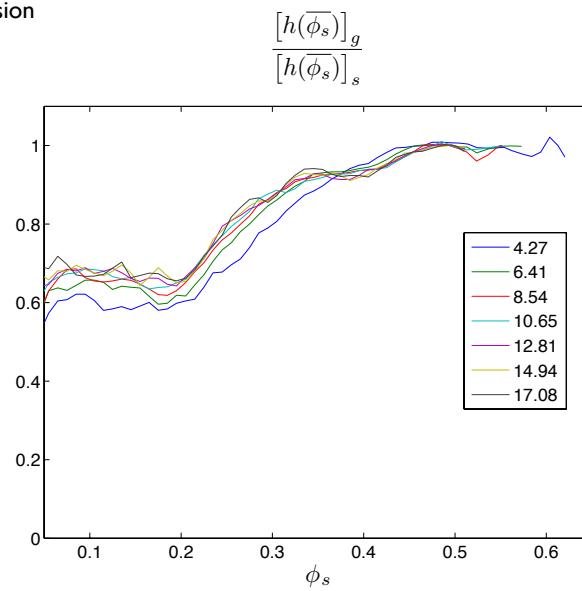
Filtered Gas Thermal Dispersion



Ratio of Gas to Solids Filtered Dispersion

$$\delta = -4/3$$

Dimensionless filter size shown in legend $\frac{\Delta}{v_t^2/g}$

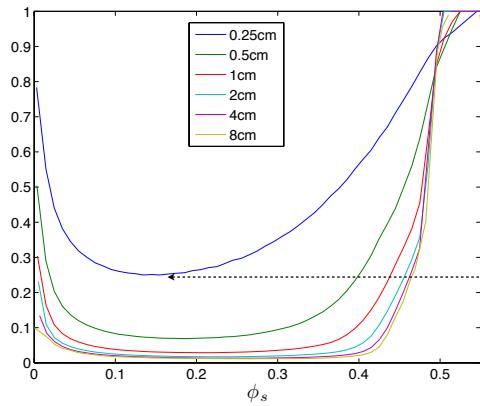


Filtered Interphase Heat Transfer Coefficient



$$\frac{\gamma_{filt}}{\gamma(\bar{\phi}_s, \tilde{v}_{slip})}$$

$$\gamma_{filt} = \frac{\gamma(T_s - T_g)}{(\bar{T}_s - \bar{T}_g)}$$



Curves correspond to
different filter sizes.

$$1 - \left[\frac{\gamma_{filt}}{\gamma(\bar{\phi}_s, \tilde{v}_{slip})} \right]_{min} \sim \left(1 + \frac{1}{[(Fr_\Delta)^{-1} - (Fr_{\Delta res})^{-1}]^+} \right)^{-0.1}$$

Dong et. al (2008); Kashyap & Gidaspow (2010,2011)

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Summary



- Filtered dispersion coefficient

$$\frac{\alpha_{filt}}{(v_t^3/g)} = \overline{\phi_s} h(\overline{\phi_s})(Fr_\Delta)^{-4/3}$$

- Filtered interphase mass/heat transfer coefficient

$$1 - \frac{\gamma_{filt}}{\gamma(\overline{\phi_s}, \tilde{v}_{slip})} \sim f(\overline{\phi_s}) \left(1 + \frac{1}{[(Fr_\Delta)^{-1} - (Fr_{\Delta res})^{-1}]^+} \right)^{-0.1}$$

Next Steps

- Explore alternate scaling

$$\frac{\alpha_{filt}}{\Delta^2 |\tilde{S}|} = G(\overline{\phi_s}) \quad |\tilde{S}| \sim \Delta^{2/3}$$

- Relate momentum dispersion to energy/scalar dispersion and interphase mass/heat transfer
- Impact of going from 2-D to 3-D

- Results for hydrodynamics suggest the effect is small (*Igci et. al, 2011*)